

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.91

Global applicability domain: Outside

Local applicability domain index: 9.33e-02

Confidence level: 8.77e-01

Nearest Neighbors from the Training Set

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N,N,N',N',N",N"-  
Hexakis(methoxymethyl)-1,3,5-  
triazine-2,4,6-triamine  
**Measured:** 3.47  
**Predicted:** 4.50

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2,5-Pyridinedicarboxylic acid  
**Measured:** 5.75  
**Predicted:** 4.09

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Docusate sodium  
**Measured:** 9.33  
**Predicted:** 8.95